

Identifiability of an Integer Modular Acyclic Additive Noise Model and its Causal Structure Discovery

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Abstract

The notion of causality is used in many situations dealing with uncertainty. We consider the problem whether causality can be identified given data set generated by discrete random variables rather than continuous ones. In particular, for non-binary data, thus far it was only known that causality can be identified except rare cases. In this paper, we present necessary and sufficient condition for an integer modular acyclic additive noise (IMAN) of two variables. In addition, we relate bivariate and multivariate causal identifiability in a more explicit manner, and develop a practical algorithm to find the order of variables and their parent sets. We demonstrate its performance in applications to artificial data and real world body motion data with comparisons to conventional methods.

Keywords: statistical causal inference, causal ordering, acyclic causal structure, integer modular variable, discrete variable

1. Introduction

We consider the problem of inferring causal relation between two random variables X, Y from a finite number of samples that have been generated

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according to the joint distribution (Spirtes et al. 2000).

Solving the problem in a general setting is rather hard, and we need some assumptions to find the causal relation: suppose X, Y are related by

$$Y = f(X) + e , \quad (1)$$

where f is a function from the range of X to that of Y , and the noise e is independent of X , and suppose further that there is no function g from the range of Y to that of X such that

$$X = g(Y) + h , \quad (2)$$

where the noise h is independent of Y . Then, we can infer that X causes Y but Y does not cause X , and say that the causality is identifiable. On the other hand, if such a function g exists, then we conclude that we cannot infer causality, and say that X, Y are reversible. This principle (additive noise model) was proposed by Shimizu et. al, who demonstrated that causality can be found if the joint distribution of X, Y is not Gaussian when f is a linear, i.e., $f(X) = aX$ with some constant a (LiNGAM) [1, 2, 3].

The same principle applies to searching (acyclic) causal relation

$$X_i = f_i(X_1, \dots, X_{i-1}) + e_i \quad (3)$$

among random variables X_1, \dots, X_i , where e_i is independent of X_1, \dots, X_{i-1} , and f_i is a linear function of X_1, \dots, X_{i-1} , $i = 1, \dots, d$. The estimated directed acyclic graph (DAG) is found from a finite number of samples [4, 5, 6]. The idea [7] is to find i and f such that

$$e_i = X_i - f(X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d)$$

is independent of $X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d$, and remove such an X_i (sink variable); starting from $S_d = \{X_1, \dots, X_d\}$, if we repeat the process (removing a sink variable from S_i to obtain S_{i-1} , $i = d-1, \dots, 1$), we obtain an order of X_1, \dots, X_d , and can rename the indexes $i = 1, \dots, d$ of X_1, \dots, X_d so that Eq. (3) holds for some f_1, \dots, f_d .

The references [8, 9, 7] address using nonlinear functions as f in Eq. (1). In another direction, [10] extended Eq. (3) to the case:

$$X_i = f_i(X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d) + e_i .$$

However, those results assumed that the random variables are continuous.

This paper addresses the case that the random variables take a finite number of values: suppose each random variable takes a value in the set $\mathcal{M} := \{0, 1, \dots, m-1\}$ for an integer $m \geq 2$, and define arithmetic over \mathcal{M} as follows: for $x, y \in \mathcal{M}$, $x + y$ takes the value $z \in \mathcal{M}$ if m divides $x + y - z$. Such a $z \in \mathcal{M}$ exists and is unique for any $x, y \in \mathcal{M}$. For example, if $m = 4$, then $3 + 2 = 1$ in $\mathcal{M} = \{0, 1, 2, 3\}$. When $m = 2$, this amounts to binary data with the exclusive-or arithmetic. Such random cyclic values are abundant in our daily life. For example, directions in $[N, E, S, W]$, months in $[1, 2, \dots, 12]$. For two random variables X, Y that take values in \mathcal{M} , we consider the additive noise model expressed by Eqs. (1)(2). The idea can be extended to the multivariate case using Eq. (3) (*integer modulus acyclic additive noise* (IMAN) model). Recently, several papers deal with such discrete cases, and we discuss those related results in the next section.

Our contributions in this paper are

1. to express necessary and sufficient conditions on causal identifiability in a bivariate IMAN model in terms of the probabilities of X and e , and
2. to develop a practical algorithm for identifying a causal structure in a multivariate IMAN model under the identifiability.

This IMAN often appears in circular/directional statistics [11, 12]. This is used in time series analysis of phase angles in the frequency domain. It has been extensively used for angular data representing an object's shape and motion as observed in ubiquitous sensing systems [13].

In Section 2, we discuss existing results related to this paper. In Section 3, we state theorems on necessary and sufficient conditions of reversibility that is equivalent to non-identifiability for a bi-variate IMAN, and show examples illustrating those theorems. These results show that the causal identifiability of an IMAN actually holds except in rare situations. In Section 4, we propose an algorithm for identifying a causal structure in a multivariate IMAN. In Sections 5 and 6, we show numerical experiments by using artificial examples and real-world data of human body motions to compare with conventional approaches, which suggests that the proposed algorithm is actually useful in many situations.

2. Related Works and Discussion

Peters et. al [14] first considered the IMAN model: let $\mathcal{M} := \{0, 1, \dots, m-1\}$ and $\mathcal{N} := \{0, 1, \dots, n-1\}$ with $m, n \geq 2$, and if we assumed X, Y take

values in \mathcal{M} and \mathcal{N} , respectively, then the causal identifiability is defined by non-existence of $g : \mathcal{N} \rightarrow \mathcal{M}$ in Eq. (2) such that h is independent of Y assuming existence of $f : \mathcal{M} \rightarrow \mathcal{N}$ in Eq. (1) such that e is independent of X .

The notions of causal identifiability and reversibility are the same even if X, Y are discrete. Let $\text{supp}(X), \text{supp}(Y), \text{supp}(e)$ be the sets of elements $x \in \mathcal{M}, y \in \mathcal{N}, y - f(x) \in \mathcal{N}$ such that $P(X = x) > 0, P(Y = y) > 0, P(e = y - f(x)) > 0$, respectively, and denote the number of elements in set A by $|A|$. They proved that for reversibility of a bivariate IMAN model, the following conditions are necessary (Theorem 4, [14]):

- (1) $|\text{supp}(Y)|$ divides $|\text{supp}(X)| \cdot |\text{supp}(e)|$.
- (2) If $|\text{supp}(X)| = m$ and $|\text{supp}(Y)| = n$, then at least one additional equality constraint on $P(X = x)$ and $P(e = y - f(x))$ over $x \in \mathcal{M}$ and $y \in \mathcal{N}$ is required.

assuming that none of X, Y, e are uniformly distributed and f is not constant.

Although the above result suggests that it is unlikely that X, Y are reversible in general situations, no essence has been captured: exactly when causality is identified for IMAN? We would be very pleased if we had a result on necessary and sufficient conditions of reversibility in terms of $P(X = x)$ and $P(e = y - f(x))$ over $x \in \mathcal{M}$ and $y \in \mathcal{N}$, respectively, and would feel safe because we would know exactly when reversibility occurs beforehand. We know that earthquakes occur very rare even in Japan but would be much happier if we knew exactly when they occur beforehand.

When $m = n$, assuming that $f : \mathcal{M} \rightarrow \mathcal{M}$ is injective, we derive the necessary and sufficient conditions in the next section. Thus far, the condition was obtained for $m = n = 2$: either $P(X = 0) = P(X = 1) = 1/2$ or $P(e = 0) = P(e = 1) = 1/2$. The condition we consider in this paper extends the existing result, and eventually, the proposed algorithm will have more applications. We notice that the assumption of injectivity can be seen in many situations including the circular/directional problems. One of the most common cases is that f is a composite function of a monotonic periodic function of discrete angles and a labeling function of the angles. This frequently appears in angle relations observed in different coordinates in mechanical sensing [13].

On the other hand, in order to establish relation between bivariate and multivariate causal identifiability, Perters et. al [15] proposed $(\mathcal{B}, \mathcal{F})$ -identifiable functional model classes (IFMOCs): Suppose that each F_i such that $X_i = F_i(X_1, \dots, X_{i-1}, e_i)$ belongs to a subset \mathcal{F} of $\{\mathbb{R}^m \rightarrow \mathbb{R} \mid \text{for some } 2 \leq m \leq d\}$. Let $\mathcal{F}_2 := \{F \in \mathcal{F} \mid F: \mathbb{R}^2 \rightarrow \mathbb{R}\}$, and \mathcal{P} the set of the distribution functions. Let \mathcal{B} be any set of $(F, F_X, F_e) \in \mathcal{F}_2 \times \mathcal{P} \times \mathcal{P}$ such that $Y = F(X, e)$, e is independent of X , and Y is not independent of X , where F_X, F_e are the distribution functions of X, e , respectively. For example, for the original LiNGAM, we may take the \mathcal{B} as the set of (F, F_X, F_e) such that $F(X, e) = aX + e$, and both of X, e should not be Gaussian. Then, they prove that if the data generated process belongs to any $(\mathcal{B}, \mathcal{F})$ -IFMOC, we can identify the exact causal graph from data (Theorem 2).

Our result in this paper does not contradict to the theorem. Instead, we show relation between bivariate and multivariate causalities in a more specific manner (Propositions 1 and 2), and propose a method to find a sink based on bivariate causality verification. More precisely, we obtain a bi-variate IMAN for any pair of variables $\{X_i, X_j\} \subset V$ by conditioning all the other variables except X_i, X_j . In fact, [15] has not addressed any method to find a sink variable uniquely from bi-variate independence relation between e_i and $\{X_j\}_{j \neq i}$ as demonstrated in DirectLiNGAM [2, 3].

On the other hand, [16] proposed a causal ordering method of binary variables. However, its identifiability is not insured, and its applicability is limited because the computational complexity is rather high.

Recently, [17] showed a necessary and sufficient condition on the bi-variate causal identifiability of Eq.(1) for binary variables. Given a value of X , $P(Y)$ coincides with either $P(e = 0)$ or $P(e = 1)$ irrespective of the value of $P(X)$. They showed the reverse model Eq.(2) satisfying the same condition among X, Y and h exists if and only if $P(e = 1) = P(e = 0)$ when $0 < P(e) < 1$. They proposed an efficient algorithm to identify a unique causal structure in a multivariate binary acyclic additive noise model named BExSAM, *i.e.*, Eq.(3) modulo 2, under the identifiability condition. However, BExSAM and its algorithm are not suitable for generic modular model. Our study indicates that a nontrivial condition different from the uniform $P(e)$ is a necessary and sufficient condition for reversibility in some generic cases, discussed in the next section, and further establishes a generic condition where a uniform $P(e)$ is a necessary and sufficient condition for reversibility.

3. Analysis on Bi-variate Identifiability

We show necessary and sufficient conditions for the reversibility of a bi-variate IMAN (1)(2), where X, Y, e take values in \mathcal{M} . For simplicity, its modulus m is a prime or its power, and $f : \mathcal{M} \rightarrow \mathcal{M}$ is injective. The notation $P(X = i) = p_i$ and $P(e = j) = q_j$ is used for brevity, and $0 < p_i < 1$ is assumed while $0 \leq q_i \leq 1$ for $i, j = 0, \dots, m-1$, which does not lose any generality since X is not constant in general situations. A typical real example arises from human body motion data demonstrated in section 6. We first present some lemmas on the reversibility for couple moduli to help understanding theorems presented later.

Lemma 1 (Reversibility For $m = 2$). *A bi-variate IMAN modulo 2 with an injective f is reversible if and only if one of the following four equalities holds: $p_1 = 1/2$, $q_1 = 1/2$, $q_1 = 0$, $q_1 = 1$.*

Proof. See Appendix Appendix A. ■

Lemma 2 (Reversibility For $m = 3$). *A bi-variate IMAN modulo 3 with an injective f is reversible if and only if one of the following five equalities holds: $p_0 = p_1 = p_2$, $q_0 = q_1 = q_2$, $q_0 = 1$, $q_1 = 1$, $q_2 = 1$.*

Proof. See Appendix Appendix B. ■

Lemma 3 (Reversibility For $m = 4$). *A bi-variate IMAN modulo 4 with an injective f is reversible if and only if either one of the following ten holds: $p_0 = p_1 = p_2 = p_3$, $q_0 = q_1 = q_2 = q_3$, $(q_0 = q_2 = 0, p_0 = p_2, p_1 = p_3)$, $(q_0 = q_2 = 0, q_1 = q_3, P_2)$, $(q_1 = q_3 = 0, p_0 = p_2, p_1 = p_3)$, $(q_1 = q_3 = 0, q_0 = q_2, P_2)$, $q_0 = 1, q_1 = 1, q_2 = 1, q_3 = 1$, where P_2 expresses the condition $(p_1/p_2 = p_3/p_0 \text{ or } p_1/p_0 = p_3/p_2)$.*

Proof. See Appendix Appendix C. ■

These lemmas are now extended to a theorem on a necessary and sufficient condition for bi-variate causal reversibility of an IMAN covering more generic moduli m . Before presenting the theorem, we need to introduce the notion of “balanced distribution” of $\{p_i\}$. We say p_0, \dots, p_{m-1} is balanced with respect

to c dividing m , if all the rows in the following matrix are identical for some constants C_0, \dots, C_{c-1} and $g : \{0, 1, \dots, c-1\} \rightarrow \{0, c, \dots, m-c\}$.

$$\begin{pmatrix} p_{0+g(0)}/C_0 & p_{0+c+g(0)}/C_0 & \dots & p_{0+m-c+g(0)}/C_0 \\ p_{1+g(1)}/C_1 & p_{1+c+g(1)}/C_1 & \dots & p_{1+m-c+g(1)}/C_1 \\ \dots & \dots & \dots & \dots \\ p_{c-2+g(c-2)}/C_{c-2} & p_{2c-2+g(c-2)}/C_{c-2} & \dots & p_{m-2+g(c-2)}/C_{c-2} \\ p_{c-1+g(c-1)}/C_{c-1} & p_{2c-1+g(c-1)}/C_{c-1} & \dots & p_{m-1+g(c-1)}/C_{c-1} \end{pmatrix}.$$

We denote the condition by P_c . For example, suppose $m = 4$ as in Lemma 3, P_2 says the rows should coincide in either

$$\begin{pmatrix} p_0/(p_0 + p_2) & p_2/(p_0 + p_2) \\ p_1/(p_1 + p_3) & p_3/(p_1 + p_3) \end{pmatrix} \text{ or } \begin{pmatrix} p_2/(p_0 + p_2) & p_0/(p_0 + p_2) \\ p_1/(p_1 + p_3) & p_3/(p_1 + p_3) \end{pmatrix},$$

corresponding to the $g : \{0, 1\} \rightarrow \{0, 2\}$ such that either $g(0) = g(1)$ or $g(0) \neq g(1)$, which is equivalent to either $p_0/p_1 = p_2/p_3$ or $p_2/p_1 = p_0/p_3$, respectively. On the other hand, we define $c(q_0, \dots, q_{m-1})$ by the smallest $c \geq 1$ such that $q_j > 0 \iff q_{j+c} > 0$. For example, for $m = 8$,

1. $q_0, \dots, q_7 > 0 \implies c(q_0, \dots, q_7) = 1$,
2. $q_0, q_2, q_4, q_6 = 0, q_1, q_3, q_5, q_7 > 0 \implies c(q_0, \dots, q_7) = 2$,
3. $q_0, q_4 = 0, q_1, q_2, q_3, q_5, q_6, q_7 > 0 \implies c(q_0, \dots, q_7) = 4$,
4. $q_j = 1$ for some $j \implies c(q_0, \dots, q_7) = 8$,
5. $q_j = 0$ for just one $j \implies c(q_0, \dots, q_7) = 8$,

and for $m = 4$ as in Lemma 3, if $q_0 = q_2 = 0$ and $q_1 = q_3$, then $c(q_0, q_1, q_2, q_3) = 2$.

Theorem 1 (Necessary and sufficient condition for reversibility). *Assume that m is a power of a prime number. Let $c := c(q_0, \dots, q_{m-1})$. Then, X and Y are reversible in a bi-variate IMAN modulo m if and only if $p_j = p_{j+c} = \dots = p_{j+m-c}$ for all $j = 0, 1, \dots, c-1$ or $(q_j = q_{j+c} = \dots = q_{j+m-c})$ for all $j = 0, 1, \dots, c-1$ and P_c .*

Proof. See Appendix Appendix D. ■

Lemmas 1 and 2 are easily derived using this theorem. Furthermore, applying $m = 4$ to this theorem, we obtain the ten conditions in Lemma 3 as follows.

Example 1 ($m = 4$).

$c = 1$: $p_0 = p_1 = p_2 = p_3$ or $q_0 = q_1 = q_2 = q_3$

$c = 2$: 1. $q_0 = q_2 = 0$ and $((p_0 = p_2 \text{ and } p_1 = p_3) \text{ or } (q_1 = q_3 \text{ and } P_2))$
 2. $q_1 = q_3 = 0$ and $((p_0 = p_2 \text{ and } p_1 = p_3) \text{ or } (q_0 = q_2 \text{ and } P_2))$

$c = 4$: $q_0 = 1$ or $q_1 = 1$ or $q_2 = 1$ or $q_3 = 1$

The following two corollaries, which are easily derived from Theorem 1, show simpler necessary and sufficient conditions under some practical assumptions.

Corollary 1. *Given a prime number m , X and Y in bivariate IMAN modulo m are reversible if and only if either of the following two conditions are met:*

$c = 1$: $p_0 = \dots = p_{m-1}$ or $q_0 = \dots = q_{m-1}$.

$c = m$: $q_k = 1$ for some k .

Proof. When m is a prime, c is either 1 or m in Theorem 1. If $c = 1$, then P_1 does not require any condition, so that Theorem 1 reads either $p_0 = \dots = p_{m-1}$ or $q_0 = \dots = q_{m-1}$. If $c = m$, which is equivalent to $q_k = 1$ for some k , no condition is required other than this. ■

Corollary 2. *Given a power of some prime number m and $q_0, \dots, q_{m-1} > 0$, X and Y in bivariate IMAN modulo m are reversible if and only if either $(p_0 = \dots = p_{m-1} \text{ or } q_0 = \dots = q_{m-1})$.*

Proof. When $q_0, \dots, q_{m-1} > 0$, which means $c = 1$ by the definition of $c(q_0, \dots, q_{m-1})$ and Theorem 1, P_1 does not require any condition. Thus, Theorem 1 reads either $p_0 = \dots = p_{m-1}$ or $q_0 = \dots = q_{m-1}$. ■

These results ensure that the causal identifiability of a bi-variate IMAN holds except for a finite number of special conditions to occur in practice. If the modulus m does not meet the condition in Theorem 1, there are some cases where the reversibility holds even if both $\{p_i\}$ and $\{q_j\}$ are nonuniform and nonzero.

Example 2 ($m = 6$). $r \geq 0$, $q_0 = q_2 = q_3 = q_5$, $q_1 = q_4 = rq_0$, $p_0 = p_2 = p_4, p_1 = p_3 = p_5 = rp_0$.

$$\begin{aligned}
R &= \begin{pmatrix} \frac{p_0q_0}{C_0} & \frac{p_1q_5}{C_0} & \frac{p_2q_4}{C_0} & \frac{p_3q_3}{C_0} & \frac{p_4q_2}{C_0} & \frac{p_5q_1}{C_0} \\ \frac{p_0q_1}{C_0} & \frac{p_1q_0}{C_0} & \frac{p_2q_5}{C_0} & \frac{p_3q_4}{C_0} & \frac{p_4q_3}{C_0} & \frac{p_5q_2}{C_0} \\ \frac{p_0q_2}{C_0} & \frac{p_1q_1}{C_0} & \frac{p_2q_0}{C_0} & \frac{p_3q_5}{C_0} & \frac{p_4q_4}{C_0} & \frac{p_5q_3}{C_0} \\ \frac{p_0q_3}{C_0} & \frac{p_1q_2}{C_0} & \frac{p_2q_1}{C_0} & \frac{p_3q_0}{C_0} & \frac{p_4q_5}{C_0} & \frac{p_5q_4}{C_0} \\ \frac{p_0q_4}{C_0} & \frac{p_1q_3}{C_0} & \frac{p_2q_2}{C_0} & \frac{p_3q_1}{C_0} & \frac{p_4q_0}{C_0} & \frac{p_5q_5}{C_0} \\ \frac{p_0q_5}{C_0} & \frac{p_1q_4}{C_0} & \frac{p_2q_3}{C_0} & \frac{p_3q_2}{C_0} & \frac{p_4q_1}{C_0} & \frac{p_5q_0}{C_0} \end{pmatrix} \\
&= \frac{p_0q_0}{r^2 + 3r + 2} \begin{pmatrix} 1 & r & r & r & 1 & r^2 \\ r & r & 1 & r^2 & 1 & r \\ 1 & r^2 & 1 & r & r & r \\ 1 & r & r & r & 1 & r^2 \\ r & r & 1 & r^2 & 1 & r \\ 1 & r^2 & 1 & r & r & r \end{pmatrix}
\end{aligned}$$

We find that X and Y are reversible by $g(0) = 0, g(1) = 4, g(2) = 2, g(3) = 0, g(4) = 4, g(5) = 2$.

In Example 2, reversibility is due to shared parameter r , which is consistent with Peters et. al [15] who suggested that reversibility requires additional equality condition among $\{p_i\}$ and $\{q_j\}$.

4. IMAN Algorithm

We assume that there exist $i \in \{1, \dots, d\}$ and f such that

$$e_i := X_i - f(\{X_j\}_{j \neq i})$$

is independent of $\{X_j\}_{j \neq i}$. In [14], we speculate that the condition (multivariate causal identifiability) reduces to bivariate causal identifiability that e_i is independent of X_j given $\{X_k\}_{k \neq i, j}$ for all $j \neq i$. We say that such X_i and a minimal subset of $\{X_j\}_{j \neq i}$ on which f depends are a *sink* and a *parent set*, respectively. In this paper, we show in Proposition 1 that the claim is true as long as the probabilities of e_i are positive. Besides, based on the strong support for bi-variate causal identifiability in Section 3 and Proposition 1, we ignore the reversible cases. From those considerations, we propose an algorithm to find a unique causal structure in an IMAN from a given modular data set D .

input: a modular data set D and $V = \{1, \dots, d\}$.

1. compute a frequency table FT for D .
2. for $k := d$ to 1 do
3. $i(k) := \mathbf{find_sink}(FT, V)$.
4. $\pi(k) := \mathbf{find_parent}(FT, V, i(k))$.
5. remove $i(k)$ from V ,
and marginalize FT with $i(k)$.
6. end

output: a list $((i(1), \pi(1)), \dots, (i(d), \pi(d)))$.

Figure 1: Main Algorithm

Figure 1 outlines the proposed algorithm which is an extension of [17] to cover the IMAN modulo $m \geq 2$. The algorithm uniquely find a sink variable, which is different from [9][15]. The first step calculates a frequency table FT from D . If we have samples of sufficiently large size, the values of relative frequency converge to the true probabilities. Steps 3 and 4 find a sink $i(k)$ and its parent set $\pi(k) \subseteq V \setminus \{i(k)\}$ given FT and V , respectively, where V is a subset of $\{1, \dots, d\}$. Step 5 removes the estimated sink $i(k)$ from V , and update FT so that the frequency values can be expressed for the updated set V excluding i (marginalization). This reduces the size of the model by one in the next cycle. The entire list $\{(i(k), \pi(k))\}_{k=1}^d$ in the output expresses a DAG structure of the IMAN.

4.1. Finding Sink and Parent Set

The proposed method is based on the following observation:

Lemma 4. 1. $X \perp\!\!\!\perp \{Y, Z\} \implies X \perp\!\!\!\perp Y|Z \wedge X \perp\!\!\!\perp Z|Y$
2. If there is no functional relation between X, Y, Z , then the converse is also true.

(Proof: see [18] for example.)

Proposition 1. Suppose X_1, \dots, X_d have no deterministic relation. Then the following conditions are equivalent:

1. X_i is a sink
2. e_i is independent of X_j given $\{X_h\}_{h \neq i, j}$ for all $j \neq i$

3. e_i is independent of $\{X_h\}_{h \neq i}$

(Proof: immediate from Lemma 4).

Proposition 1 implies that we can check that X_i is a sink by verifying e_i to be independent of $\{X_h\}_{h \neq i}$, and that finding the sink node is as likely as bivariate causal identifiability.

In `find_sink`, the conditional probability $P(X_i = x_i | \{X_j = x_k\}_{j \neq i})$ is estimated from FT (we write the value by $\hat{P}(X_i = x_i | \{X_j = x_k\}_{j \neq i})$). Suppose that X_i is a sink node. Then, the probability of $e_i = X_i - f(\{X_j\}_{j \neq i})$ is the same for $\{X_j = x'_j\}_{j \neq i}$ and $\{X_j = x''_j\}_{j \neq i}$. If we choose x'_i and x''_i such that $\hat{P}(X_i = x'_i | \{X_j = x'_k\}_{j \neq i})$ and $\hat{P}(X_i = x''_i | \{X_j = x''_k\}_{j \neq i})$ are maximized, respectively. Then, it is likely that

$$x'_i - x''_i = f(\{x'_j\}_{j \neq i}) - f(\{x''_j\}_{j \neq i}) \quad (4)$$

if the sample size n is large. Let c be the value of (4). Then, the distributions of X_i and $X_i + c$ given $\{X_j = x'_j\}_{j \neq i}$ and $\{X_j = x''_j\}_{j \neq i}$, respectively, should be the same if the estimation of c is correct.

To this end, we apply the data to the G-test [19] which distinguishes whether $P(\cdot|A) = P(\cdot|B)$ or not for disjoint events A, B from data. The G-test calculates the G-value:

$$\begin{aligned} & 2 \sum_k c_n(C_k \cap A) \log \left\{ \frac{c_n(C_k \cap A)}{c_n(A)} / \frac{c_n(C_k)}{n} \right\} \\ & + 2 \sum_k c_n(C_k \cap B) \log \left\{ \frac{c_n(C_k \cap B)}{c_n(B)} / \frac{c_n(C_k)}{n} \right\}, \end{aligned} \quad (5)$$

where $c_n(\cdot)$ is the frequency of the event, and $\{C_k\}$ are disjoint events covering the whole events ($\cup_k C_k = \Omega$). The G-test is more correct than the χ^2 -test that calculates an approximation of (5). In our case, in order to prove Independence, we compare the values $\hat{P}(\cdot | \{X_j = x_j\}_{j \neq i})$ for all $\{x_j\}_{j \neq i}$ in \mathcal{M}^{d-1} .

Once the sink $i(k)$ is obtained, we find the parent set $\pi(k) \subseteq V \setminus \{i\}$ assuming that the estimated $i(k)$ is correct. We find the parent based on the following observation:

Proposition 2. Suppose X_1, \dots, X_d have no deterministic relation. Then, for any $i \in V := \{1, \dots, d\}$ and $\pi \subseteq V - \{i\}$,

$$X_i \perp\!\!\!\perp X_j | \{X_h\}_{h \neq i, j}, j \in V - \pi - \{i\} \iff X_i \perp\!\!\!\perp \{X_j\}_{j \in V - \pi - \{i\}} | \{X_h\}_{h \in \pi}$$

(Proof: immediate from Lemma 4). To this end, for each $j \neq i(k)$, we compute $\hat{P}(X_{i(k)}, X_j | \{X_h = x_h\}_{h \neq i(k), j})$ for all $\{x_h\}_{h \neq i(k), j} \in \mathcal{M}^{d-2}$ to test if $X_{i(k)}$ and X_j are independent via the G-test given $\{X_h = x_h\}_{h \neq i(k), j}$. We see that $j \in \pi(k)$ if and only if $X_{i(k)}$ and X_j are not independent given at least one $\{x_h\}_{h \neq i(k), j} \in \mathcal{M}^{d-2}$. We test all the tables of $\{x_h\}_{h \neq i(k), j} \in \mathcal{M}^{d-2}$ by multiple comparison tests [20]. Throughout this paper, `find_parent` uses the significance level $\alpha = 0.05$ and repeats the procedure for all $j \neq i(k)$ to enumerate all the values of $\pi(k)$.

4.2. Computational Complexity

The table `FT` is of size m^d . Hence, the space complexity is $O(m^d)$. The critical task in `find_sink` is to compute $m \times m^{d-1}$ conditional probability tables for $i(k)$, and this is repeated at most d times. The critical task in `find_parent` is the m^{d-2} times computation of $m \times m$ conditional probability tables for $j \neq i(k)$, and this is repeated $d-1$ times at most. These are further repeated d times in the main algorithm shown in Fig.1. Accordingly, the total time complexity is $O(d^2 m^d)$. We require that the data size n is near the size of `FT`, i.e., m^d . Therefore, when $n \simeq m^d$, the complexity is virtually $O(d^2 n)$ which is comparable or better than previous work. For example, `DirectLiNGAM` [2, 3] which is one of the most efficient causal inference algorithm requires $O(d^3 n)$.

5. Experimental Evaluation

In this section, we evaluate the basic performance of our algorithm by using artificial data. Let d be the number of variables $\{X_i\}_{i=1}^d$, m the size of the modulus domain \mathcal{M} , n the number of samples, p_a the probability that X_i is a parent of X_j for each $i \neq j$, and $\{q_i\}_{i=0}^{m-1}$ with $\sum_{i=0}^{m-1} q_i = 1$ the noise distribution. For each sink i with parent set π , f_i is a function of $\{X_j\}_{j \in \pi}$. We add noise e_i to $f_i(\{x_j\}_{j \in \pi})$ to obtain $X_i = x_i$ given $\{X_j = x_j\}_{j \in \pi}$. By repeating the process for $i = 1, \dots, d$, we obtain one realization $\{X_i = x_i\}_{i=1}^d$. For simplicity, we assume that all the noise $\{e_i\}_{i=1}^d$ share the same distribution. Furthermore, by generating $\{X_i = x_i\}_{i=1}^d$ n times and randomly changing the indexes $(i)_{1 \leq i \leq d}$ of $\{X_i\}_{i=1}^d$ into some $(i(k))_{1 \leq k \leq d}$, we obtain data set D . In our experiments, we estimate $\{i(k), \pi(k)\}_{k=1}^d$ from the data set D obtained above.

We evaluate performance of IMANN in terms of several measures. Suppose we estimate $\{i(k), \pi(k)\}_{k=1}^d$ to obtain $\{\hat{i}(k), \hat{\pi}(k)\}_{k=1}^d$ from D . Then, we can obtain the adjacency matrices B and \hat{B} for $\{i(k), \pi(k)\}_{k=1}^d$ and

Table 1: Performance under various d and m .

$d \backslash m$	2	3	4	5	6
2	0.033	0.011	0.006	0.004	0.000
	0.958	0.973	0.985	0.985	1.000
	0.741	0.740	0.766	0.803	0.960
4	0.040	0.016	0.014	0.034	0.005
	0.941	0.957	0.958	0.933	0.967
	2.66	2.97	3.65	5.24	116.4
6	0.036	0.031	0.211	0.317	0.093
	0.927	0.921	0.785	0.747	0.844
	5.57	10.3	8.3	128.0	8736.
8	0.050	0.228	0.338	0.351	0.247
	0.898	0.766	0.744	0.748	0.793
	11.2	86.0	722.	4476.	552060.

Top:*Ero*, Middle:*Acc* and Bottom:*CT* in a cell.
 q_i are uniformly random.

$\{\hat{i}(k), \hat{\pi}(k)\}_{k=1}^d$, respectively. If we change the orders of rows and columns so that the matrix B becomes lower triangular, the matrix \hat{B} does not become lower triangular unless the estimation is correct. Let $UT(B, \hat{B})$ be the number of nonzero elements in the upper triangular in \hat{B} . Then, we define *Ero* by

$$Ero = \frac{UT(B, \hat{B})}{d(d-1)/2},$$

which expresses the ratio of the number of inconsistent edges to the number of the whole possible edges. This measure has been used in many studies including LiNGAM [1]. We also evaluate in how many elements B and \hat{B} coincide, i.e., the ratio of the number of elements matched between B and \hat{B} to the number of the whole elements except the diagonal elements, $d(d-1)$. This measure (*Acc*) expresses accuracy of the estimated causal structure. (The less *Ero* and the larger *ACC*, the better performance.) We also evaluate computation time *CT* (msec) which expresses its algorithm scalability. We randomly executed 1000 trials and took average among them. For the experiments, we installed MATLAB R2011a on a Windows 7 machine with Xeon W3565 (3.2GHz, 4 core, 8MB cache), 6GB RAM and 500GB HDD.

Table 2: Performance under various d and m .

$d \backslash m$	2	3	4	5	6
2	0.014	0.011	0.006	0.008	0.160
	0.976	0.989	0.989	0.991	0.840
4	0.020	0.031	0.013	0.012	0.273
	0.959	0.957	0.947	0.946	0.763
6	0.025	0.058	0.028	0.033	0.261
	0.944	0.909	0.901	0.895	0.781
8	0.044	0.148	0.079	0.092	0.290
	0.913	0.788	0.825	0.812	0.765

Top:*Ero* and Bottom:*Acc* in a cell.

Two adjacent q_i and q_{i+1} are respectively p and $1 - p$.

Based on the result in section 4, we are particularly interested in the effects of m and $\{q_i\}_{i=0}^{m-1}$ on the estimation accuracy. The parameter d is also an important factor for scalability. Table 1 shows the results under which each $0 < q_i < 1$ is set uniformly random, $n = 1000$, $p_a = 0.5$. In this case, $\{q_i\}_{i=0}^{m-1}$ can be mutually close by chance when m , is small. According to our Theorem 1 and Corollary 2, such a condition violates the bi-variate causal identifiability of the IMAN. However, the chance is reduced as m grows. This is reflected in *Ero* and *Acc* when $m = 5$ and 6. Although $m = 6$ is not a power of a prime number, its causal identifiability holds similarly to the other numbers. This is consistent with the observation in Example 2 and [14].

On the other hand, if m is large, the size of frequency table FT relative to n is large, and we might not have enough samples to estimate the conditional probabilities from D via the G-test. Because the FT size is $O(m^d)$, the critical size n of D should be at least m^d to compute statistically accurate FT . For example, the errors can be seen to be significantly large when $(d, m) = (6, 4), (8, 3)$ ($m^d > n = 1000$). On the other hand, from Table 1, our algorithm seems to provide practical accuracy if n is larger than m^d . Also, we find that CT reflects $O(d^2 m^d)$ of the algorithm as analyzed in Section 4.2. Table 2 indicates the results when $q_i = p$, $q_{i+1} = 1 - p$, $q_j = 0$, $j \neq i, i + 1$ for $0 < p < 1$, $n = 1000$, and $p_a = 0.5$. In this case, $\{p_i\}_{i=0}^{m-1}$ are always far from any reversible conditions shown in our theorem and corollaries. Thus, it is reasonable to think that accuracy is obtained as long as n is large enough

Table 3: Performance under various n .

n	100	500	1000	5000	10000
Ero	0.218	0.037	0.014	0.003	0.001
Acc	0.769	0.923	0.958	0.982	0.983

q_i is uniformly random, $d=4$ and $m = 4$.

Table 4: Performance under various p_a .

p_a	0.0	0.2	0.4	0.6	0.8	1.0
Ero	0.000	0.005	0.012	0.016	0.020	0.023
Acc	0.964	0.961	0.963	0.958	0.957	0.952

q_i is uniformly random, $d = 4$ and $m = 4$.

compared with m^d .

Table 3 and 4 show the performance in terms of n and p_a under $d = 4$, $m = 4$, and uniform q_i . The error is reduced as n grows. However, again we observe the critical size of n is $n \simeq m^d$. When p_a is large (the structure is dense), wrong selection of a sink variable in causal ordering affects the ordering of all the remaining variables. Therefore, *Ero* increases as density grows whereas *Acc* does not decrease.

6. Real-world Applications

We analyzed human body orientation data of MPI08_Database² [13]. Various indoor motions of a human measured with eight movie cameras and five orientation sensors are stored in the data. Five angle sensors are attached to various parts of the body between knees and ankles, between wrists and hands and between chest and neck, and angles measured with respect to a global inertial coordinate frame at 40Hz which is suitable to describe human body orientation in his/her view. We obtained angles $[roll, pitch, yaw]$ from each snapshot output: *roll* is the rotation angle around the rotation axis;

²The data is accessible at http://www.tnt.uni-hannover.de/project/MPI08_Database/.

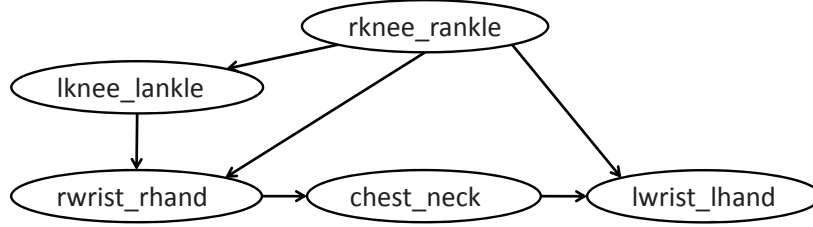


Figure 2: A Causal Network (IMAN, *roll*).

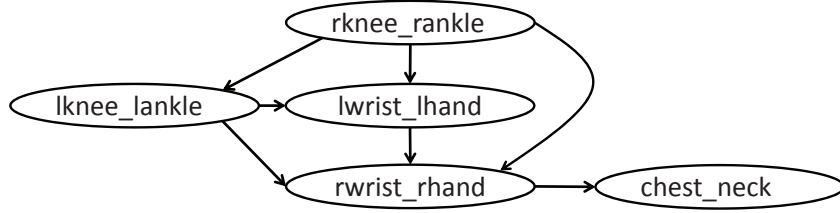


Figure 3: A Causal Network (IMAN, *roll*, Cartwheel).

pitch is the look up angle between the axis and a horizontal plain; and *yaw* is the horizontal direction angle of the axis. *roll* and *yaw* take cyclic values in $[0, 2\pi)$, whereas *pitch* takes values in $[-\pi/2, +\pi/2]$.

We applied our IMAN algorithm to *roll* of the data sets; “ab_01_01” and “ab_10_01.” The former records a counterclockwise walking motion over 406 time steps. The latter records two cartwheel motions over 580 time steps, and we analyzed the first 200 time steps on the leftward cartwheel motion. We discretized each *roll* into 3 equi-width intervals of $[-\pi, -\pi/6)$, $[-\pi/6, +\pi/6)$, $[+\pi/6, +\pi)$. The critical $m^d = 3^5 = 243$ is comparable with $n = 406$ and 200 for both data sets. Figure 2 shows a causal network on ab_01_01 by the IMAN algorithm. This result is well interpreted in that the right leg, its orientation being measured by rknee_rankle sensor, takes the initiative, and the left leg and right hand, as measured by lknee_lankle and rwrist_rhand sensors respectively, follow the right leg motion, and are further followed by the neck and left hand, as measured by chest_neck and lwrist_lhand sensors respectively. Figure 3 shows the result on ab_10_01. To initiate the leftward cartwheel, the right leg is used first to push off from the floor. The motion then influences the orientation of his left leg, and subsequently planting of these left hand on the floor hand to support the body in the rotation. In

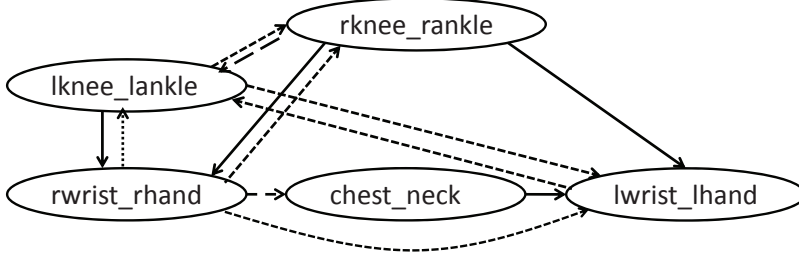


Figure 4: A Causal Network (VAR, *pitch*).

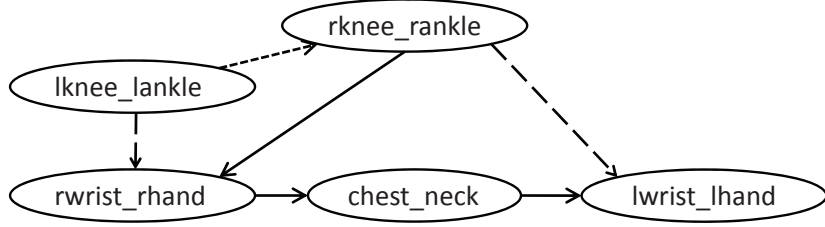


Figure 5: A Causal Network (DirectLiNGAM, *pitch*).

turn, the right hand is planted in similar manner as the body continues to rotate. The neck always follows these motions to maintain body balance.

Because these are time series representing the body motion dynamics, we also applied VAR (Vector Auto-Regressive) (Fig. 4) [21] and DirectLiNGAM (Fig. 5) [2, 3] to *pitch* by assuming *pitch* shares similar causality with *roll*, because no approaches are applicable to the modular *roll*. We used the 1st order VAR model selected by the final prediction error (FPE) in Fig. 4. In both figures, the causal networks are drawn by the matrix elements above a certain threshold level. The dotted edges are outputs of VAR and DirectLiNGAM that is not in the IMAN output; the dashed edges are the output of IMAN but not in the others. Though VAR indicates cycles, 4 out of 6 edges of IMAN are supported. DirectLiNGAM's causal order is consistent except lknee_lankle. Though these are not from *roll*, they are quite consistent with IMAN. We analyzed some other data obtained from kicking motions, and produced a similar consistency.

7. Discussion and Conclusion

In this paper, we presented necessary and sufficient conditions for bivariate causal identifiability in IMAN, and actually affirm that causality can be identified except in rare cases. Our result locates exactly when the reversible cases occur. In addition, we relate bivariate and multivariate causal identifiability in more precise manner for IMANN (Propositions 1 and 2).

As a result, we developed a practical way to find a sink and its parent set. The algorithm needs a sufficient number of samples compared with m^d to verify independence when each of X_1, \dots, X_d takes a value among m values. The computational complexity is $O(d^2 m^d)$, and it is reasonable to say that the value d should be at most 10 for small m , which is according to our experiments in this paper (the value m can be small in practical situations by reducing the quantization level).

If the sample size n is small, we need to improve estimation of FT. One possibility is to construct a Bayesian measure to deal with each sample set, and we expect to obtain more robust results even for small m . Then, we can avoid checking independence via the G-test.

The most important direction for future study is to seek a causal model and its causal identifiability conditions on continuous and cyclic data, such as that used in section 6. If we address these issues, our approach can be extended so that we do not need to discretize these data to integers. Recent studies in directional statistics provided some analyses on distributions of circular/directional variables [11, 12].

Appendix A. Proof of Lemma 1

There are four functions $f : \mathcal{M} \rightarrow \mathcal{M}$, where only $f(X) = X$ and $f(X) = X + 1$ are injective. Let $P(X|Y)$ be such that

$$P(X|Y) := \begin{pmatrix} P(X=0|Y=0) & P(X=1|Y=0) \\ P(X=0|Y=1) & P(X=1|Y=1) \end{pmatrix}. \quad (\text{A.1})$$

If X and Y are reversible, there exists $g : \mathcal{M} \rightarrow \mathcal{M}$ such that $X = g(Y) + h$, $Y \perp\!\!\!\perp h$, which is equivalent to $P(h) = P(h|Y) = P(X - g(Y)|Y)$. Accordingly,

$$P(h) := \begin{pmatrix} P(X - g(0) = 0|Y=0) & P(X - g(0) = 1|Y=0) \\ P(X - g(1) = 0|Y=1) & P(X - g(1) = 1|Y=1) \end{pmatrix},$$

where the first and second rows are mutually identical. Note that the upper row is equal to the upper row cyclically shifted to the left by $g(0)$ in Eq.(A.1) whereas the lower row is the $g(1)$ cyclical left shift of the lower row in Eq.(A.1). If $g(Y) = Y$, this condition is equivalent to

$$P(h) := \begin{pmatrix} P(X=0|Y=0) & P(X=1|Y=0) \\ P(X=1|Y=1) & P(X=0|Y=1) \end{pmatrix}. \quad (\text{A.2})$$

If $g(Y) = Y + 1$, $P(h)$ is equal to the matrix in which $X = 0$ and $X = 1$ are exchanged in the above. If $g(Y) = 0$,

$$P(h) := \begin{pmatrix} P(X=0|Y=0) & P(X=1|Y=0) \\ P(X=0|Y=1) & P(X=1|Y=1) \end{pmatrix}, \quad (\text{A.3})$$

and if $g(Y) = 1$, $P(h)$ is equal to the matrix in which $X = 0$ and $X = 1$ are exchanged in the above.

To establish the proof, we first consider the case $q_1 \neq 0, 1$. For $f(X) = X$, if X and Y are reversible under $g(Y) = Y$, the two rows in Eq.(A.2) are mutually identical:

$$\begin{aligned} & \left(\frac{(1-p_1)(1-q_1)}{(1-p_1)(1-q_1) + p_1q_1}, \frac{p_1q_1}{(1-p_1)(1-q_1) + p_1q_1} \right) \\ &= \left(\frac{p_1(1-q_1)}{(1-p_1)q_1 + p_1(1-q_1)}, \frac{(1-p_1)q_1}{(1-p_1)q_1 + p_1(1-q_1)} \right) \\ &\iff p_1 = 1/2. \end{aligned}$$

Under $g(Y) = Y + 1$, $p_1 = 1/2$ is obtained as well. When $g(Y) = 0$, the two rows in Eq.(A.3) are identical:

$$\begin{aligned} & \left(\frac{(1-p_1)(1-q_1)}{(1-p_1)(1-q_1) + p_1q_1}, \frac{p_1q_1}{(1-p_1)(1-q_1) + p_1q_1} \right) \\ &= \left(\frac{(1-p_1)q_1}{(1-p_1)q_1 + p_1(1-q_1)}, \frac{p_1(1-q_1)}{(1-p_1)q_1 + p_1(1-q_1)} \right) \\ &\iff q_1 = 1/2. \end{aligned}$$

For $g(Y) = 1$, $q_1 = 1/2$ is obtained as well. For $f(X) = X + 1$, the matrices $P(h)$ are the same as that for $f(X) = X$ except that the order of the two rows is reversed. Hence, the same result is obtained. Thus, as long as f is injective and $0 < q_1 < 1$, the reversibility requires either $p_1 = 1/2$ or $q_1 = 1/2$.

If $q_1 = 0, 1$, meaning $Y = f(X)$ and $Y = f(X) + 1$, respectively, X and Y are reversible for injective f such as $f(X) = X$ and $f(X) = X + 1$. ■

Appendix B. Proof of Lemma 2

For injective $f : \mathcal{M} \rightarrow \mathcal{M}$, we wish to find $g : \mathcal{M} \rightarrow \mathcal{M}$ such that $Y = f(X) + e$ and $h := X - g(Y)$ are independent. To this end, $P(h) = P(h|Y) = P(X - g(Y)|Y)$ is obtained by cyclic left $g(Y)$ shift of each row in the following $P(X|Y)$ to find such g .

$$P(X|Y) := \begin{pmatrix} P(X=0|Y=0) & P(X=1|Y=0) & P(X=2|Y=0) \\ P(X=0|Y=1) & P(X=1|Y=1) & P(X=2|Y=1) \\ P(X=0|Y=2) & P(X=1|Y=2) & P(X=2|Y=2) \end{pmatrix}.$$

For example, when $g(Y) = Y$,

$$\begin{aligned} P(h) &= P(h|Y) \\ &= \begin{pmatrix} P(h=0|Y=0) & P(h=1|Y=0) & P(h=2|Y=0) \\ P(h=0|Y=1) & P(h=1|Y=1) & P(h=2|Y=1) \\ P(h=0|Y=2) & P(h=1|Y=2) & P(h=2|Y=2) \end{pmatrix} \\ &= P(X - g(Y)|Y) = P(X - Y|Y) \\ &= \begin{pmatrix} P(X=0|Y=0) & P(X=1|Y=0) & P(X=2|Y=0) \\ P(X=1|Y=1) & P(X=2|Y=1) & P(X=0|Y=1) \\ P(X=2|Y=2) & P(X=0|Y=2) & P(X=1|Y=2) \end{pmatrix} \end{aligned}$$

where the 0th row is a 0 shift of the 0th row of $P(X|Y)$, the 1st row is a cyclic left 1 shift of the 1st row of $P(X|Y)$, and the 2nd row is a cyclic left 2 shift of the 2nd row of $P(X|Y)$. However, for ease of notation, we consider the following table

$$P(f(X)|Y) = \begin{pmatrix} P(f(X)=0|Y=0) \\ P(f(X)=0|Y=1) \\ P(f(X)=0|Y=2) \\ P(f(X)=1|Y=0) & P(f(X)=2|Y=0) \\ P(f(X)=1|Y=1) & P(f(X)=2|Y=1) \\ P(f(X)=1|Y=2) & P(f(X)=2|Y=2) \end{pmatrix}.$$

Generality is not lost because f must be injective. Hereafter, we find $g : \mathcal{M} \mapsto \mathcal{M}$ such that $f(X) - g(Y)$ and Y are independent. Let

$$R = P(f(X)|Y) = (r_{k,i})$$

such that

$$r_{k,i} := P(f(X) = i | Y = k) = \frac{p_i q_{k-i}}{\sum_j p_j q_{k-j}},$$

where $e = Y - f(X) = k - i$ and $f(X) \perp\!\!\!\perp e$. Thus,

$$R = \begin{pmatrix} p_0 q_0 / C_0 & p_1 q_2 / C_0 & p_2 q_1 / C_0 \\ p_0 q_1 / C_1 & p_1 q_0 / C_1 & p_2 q_2 / C_1 \\ p_0 q_2 / C_2 & p_1 q_1 / C_2 & p_2 q_0 / C_2 \end{pmatrix},$$

where $C_0 = p_0 q_0 + p_1 q_2 + p_2 q_1$, $C_1 = p_0 q_1 + p_1 q_0 + p_2 q_2$, and $C_2 = p_0 q_2 + p_1 q_1 + p_2 q_0$.

First of all, we consider the case $q_0, q_1, q_2 > 0$. We find conditions that X and Y are reversible for each of the nine cases $\{(i, j) \in \mathcal{M}^2 | g(1) = g(0) + i, g(2) = g(0) + j\}$. If $g(1) = g(0)$, the 0th and the 1st rows in R are equally cyclic left-shifted by $g(0) = g(1)$, and thus $p_0 q_0 / C_0 = p_0 q_1 / C_1$, $p_1 q_2 / C_0 = p_1 q_0 / C_1$, and $p_2 q_1 / C_0 = p_2 q_2 / C_1$. These yield

$$\frac{p_0 q_0}{p_0 q_1} = \frac{p_1 q_2}{p_1 q_0} = \frac{p_2 q_1}{p_2 q_2} \iff q_0 = q_1 = q_2.$$

If $g(1) = g(0) + 1$, we cyclically shift the 1st row to the left by one column to compare with the 0th row. This yields

$$\frac{p_0 q_0}{p_1 q_0} = \frac{p_1 q_2}{p_2 q_2} = \frac{p_2 q_1}{p_0 q_1} \iff p_0 = p_1 = p_2.$$

If $g(1) = g(0) + 2$, we cyclically shift the 1st row to the left by two columns to compare with the 0th row and obtain

$$\frac{p_0 q_0}{p_2 q_2} = \frac{p_1 q_2}{p_0 q_1} = \frac{p_2 q_1}{p_1 q_0} = C_0 / C_1.$$

By taking a product of these three terms, we obtain $(C_0 / C_1)^3 = 1$. Thus,

$$\frac{p_0 q_0}{p_2 q_2} = \frac{p_1 q_2}{p_0 q_1} = \frac{p_2 q_1}{p_1 q_0} = 1. \tag{B.1}$$

Similarly, if we compare the 0th and 2nd rows, we obtain

$$\begin{aligned} \frac{p_0 q_0}{p_0 q_2} = \frac{p_1 q_2}{p_1 q_1} = \frac{p_2 q_1}{p_2 q_0} &\iff q_0 = q_1 = q_2, \\ \frac{p_0 q_0}{p_1 q_1} = \frac{p_1 q_2}{p_2 q_0} = \frac{p_2 q_1}{p_0 q_2} &= 1, \end{aligned} \tag{B.2}$$

and

$$\frac{p_0 q_0}{p_2 q_0} = \frac{p_1 q_2}{p_0 q_2} = \frac{p_2 q_1}{p_1 q_1} \iff p_0 = p_1 = p_2$$

for $g(2) = g(0)$, $g(2) = g(0) + 1$, and $g(2) = g(0) + 2$, respectively. For the eight cases $(i, j) = (0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2), (2, 0)$ and $(2, 2)$, we immediately find $p_0 = p_1 = p_2$ or $q_1 = q_2 = q_3$. Alternatively, for $(i, j) = (2, 1)$, we combine equations (B.1) and (B.2). By taking products of two terms taken from each equation to cancel out q_i , we obtain $p_1 p_2 / p_0^2 = 1 \iff p_0^3 = p_0 p_1 p_2$ and similarly $p_1^3 = p_0 p_1 p_2$, $p_2^3 = p_0 p_1 p_2$ which give $p_0 = p_1 = p_2$. We also obtain $q_0 = q_1 = q_2$ in the same way. If we substitute either $p_0 = p_1 = p_2$ or $q_0 = q_1 = q_2$ into the table R , we can easily find cyclic left-shifts to make all rows identical. In summary, there exists g for the reversibility under $q_1, q_2, q_3 > 0$, if and only if any of $p_0 = p_1 = p_2$ or $q_1 = q_2 = q_3$ hold.

On the other hand, suppose just one of q_0, q_1, q_2 is zero. For instance, if $q_0 = 0$, q_0 should appear in the same column to make the rows identical by the cyclic shift $(i, j) = (1, 2)$ and

$$\frac{p_1 q_2}{p_2 q_2} = \frac{p_2 q_1}{p_0 q_1}, \frac{p_1 q_2}{p_0 q_2} = \frac{p_2 q_1}{p_1 q_1} \iff p_0 = p_1 = p_2$$

is obtained. Similarly, $p_0 = p_1 = p_2$ is required for each of $(q_0 = 0, q_1 \neq 0, q_2 \neq 0)$, $(q_0 \neq 0, q_1 = 0, q_2 \neq 0)$, $(q_0 \neq 0, q_1 \neq 0, q_2 = 0)$.

Suppose just two of q_0, q_1, q_2 are zero. From $q_0 + q_1 + q_2 = 1$, one of $q_0 = 1, q_1 = 1$ and $q_2 = 1$ holds. Thus,

$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},$$

hold respectively. Under cyclic left $g(Y)$ shifting by $(i, j) = (1, 2)$, the three rows in every R become identical. Thus, reversibility holds. \blacksquare

Appendix C. Proof of Lemma 3

We denote

$$R = \begin{pmatrix} p_0 q_0 / C_0 & p_1 q_3 / C_0 & p_2 q_2 / C_0 & p_3 q_1 / C_0 \\ p_0 q_1 / C_1 & p_1 q_0 / C_1 & p_2 q_3 / C_1 & p_3 q_2 / C_1 \\ p_0 q_2 / C_2 & p_1 q_1 / C_2 & p_2 q_0 / C_2 & p_3 q_3 / C_2 \\ p_0 q_3 / C_3 & p_1 q_2 / C_3 & p_2 q_1 / C_3 & p_3 q_0 / C_3 \end{pmatrix}.$$

Suppose that we have a table T such that all rows are identical by cyclically shifting the k -th row left by $g(k)$ columns in the table.

First of all, we consider the case $q_0, q_1, q_2, q_3 > 0$. If the indices i of p_i coincide in more than one row in T , we have some of the following conditions.

$$\begin{aligned} \frac{p_0 q_0}{p_0 q_1} = \frac{p_1 q_3}{p_1 q_0} = \frac{p_2 q_2}{p_2 q_3} = \frac{p_3 q_1}{p_3 q_2} &\iff q_0 = q_1 = q_2 = q_3, \\ \frac{p_0 q_0}{p_0 q_2} = \frac{p_1 q_3}{p_1 q_1} = \frac{p_2 q_2}{p_2 q_0} = \frac{p_3 q_1}{p_3 q_3} &\iff q_0 = q_2, q_1 = q_3, \\ \frac{p_0 q_0}{p_0 q_3} = \frac{p_1 q_3}{p_1 q_2} = \frac{p_2 q_2}{p_2 q_1} = \frac{p_3 q_1}{p_3 q_0} &\iff q_0 = q_1 = q_2 = q_3, \\ \frac{p_0 q_1}{p_0 q_2} = \frac{p_1 q_0}{p_1 q_1} = \frac{p_2 q_3}{p_2 q_0} = \frac{p_3 q_2}{p_3 q_3} &\iff q_0 = q_1 = q_2 = q_3, \\ \frac{p_0 q_1}{p_0 q_3} = \frac{p_1 q_0}{p_1 q_2} = \frac{p_2 q_3}{p_2 q_1} = \frac{p_3 q_2}{p_3 q_0} &\iff q_0 = q_2, q_1 = q_3, \\ \frac{p_0 q_2}{p_0 q_3} = \frac{p_1 q_1}{p_1 q_2} = \frac{p_2 q_0}{p_2 q_1} = \frac{p_3 q_3}{p_3 q_0} &\iff q_0 = q_1 = q_2 = q_3. \end{aligned}$$

Suppose $q_0 = q_2, q_1 = q_3$. Then, we have

$$R = \begin{pmatrix} p_0 q_0 / C_0 & p_1 q_1 / C_0 & p_2 q_0 / C_0 & p_3 q_1 / C_0 \\ p_0 q_1 / C_1 & p_1 q_0 / C_1 & p_2 q_1 / C_1 & p_3 q_0 / C_1 \end{pmatrix}$$

written by excluding the identical rows. If the 1st row cyclically shifted left by 0, 1, 2, 3 columns is identical to the 0th row, we obtain $q_0 = q_1 = q_2 = q_3$, $p_0 = p_1 = p_2 = p_3$, $(p_0 = p_2, p_1 = p_3)$, $p_0 = p_1 = p_2 = p_3$, respectively. If $p_0 = p_2, p_1 = p_3$, then, by excluding the identical columns,

$$R = \begin{pmatrix} p_0 q_0 / C_0 & p_1 q_1 / C_0 \\ p_0 q_1 / C_1 & p_1 q_0 / C_1 \end{pmatrix} \iff q_0 = q_1 \text{ or } p_0 = p_1$$

upon cyclically shifting left by 0 or 1 respectively. Thus, in any eventuality, $p_0 = p_1 = p_2 = p_3$ or $q_0 = q_1 = q_2 = q_3$ ensure the existence of g for reversibility. From the symmetry of $\{p_i\}$ and $\{q_j\}$, the results where $\{p_i\}$ and $\{q_j\}$ are exchanged are obtained even when the indices j of q_j coincide in more than one row in T .

Hence, without loss of generality, we compare rows such that no i of p_i and j of q_j are the same in any two rows in T . For two rows $k, l = 0, 1, 2, 3$, there exist columns i, j such that $i \neq j$, $k - i \neq l - j$ and

$$\frac{p_i q_{k-i}}{p_j q_{l-j}} = \frac{p_{i+1} q_{k-i-1}}{p_{j+1} q_{l-j-1}} = \frac{p_{i+2} q_{k-i-2}}{p_{j+2} q_{l-j-2}} = \frac{p_{i+3} q_{k-i-3}}{p_{j+3} q_{l-j-3}}$$

for the identity. If we fix k and multiply the terms over rows $l = 0, 1, 2, 3$ vertically under the identity of all rows for the reversibility, we obtain

$$\frac{[p_i q_{k-i}]^4}{\prod_u p_u \prod_v q_v} = \frac{[p_{i+1} q_{k-i-1}]^4}{\prod_u p_u \prod_v q_v} = \frac{[p_{i+2} q_{k-i-2}]^4}{\prod_u p_u \prod_v q_v} = \frac{[p_{i+3} q_{k-i-3}]^4}{\prod_u p_u \prod_v q_v}$$

where all the denominators are the same since no i of p_i and j of q_j are the same in any two rows in T and $(i, k-i)$ and $(j, l-j)$ are different for each of $k, l = 0, 1, 2, 3$. Thus,

$$p_i q_{k-i} = p_{i+1} q_{k-i-1} = p_{i+2} q_{k-i-2} = p_{i+3} q_{k-i-3}$$

are constant. If we sum over the terms over $k = 0, 1, \dots, 3$, we obtain $p_i = p_{i+1} = p_{i+2} = p_{i+3}$, thus both $p_0 = p_1 = p_2 = p_3$ and $q_0 = q_1 = q_2 = q_3$ are required for reversibility.

Suppose just one of the q_0, q_1, q_2, q_3 are zero. If $q_0 = 0$, R is cyclically shifted to be the following S , where all the rows are identical for the reversibility.

$$\begin{aligned} S &= \begin{pmatrix} 0 & q_3 p_1 / C_0 & q_2 p_2 / C_0 & q_1 p_3 / C_0 \\ 0 & q_3 p_2 / C_1 & q_2 p_3 / C_1 & q_1 p_0 / C_1 \\ 0 & q_3 p_3 / C_2 & q_2 p_0 / C_2 & q_1 p_1 / C_2 \\ 0 & q_3 p_0 / C_3 & q_2 p_1 / C_3 & q_1 p_2 / C_3 \end{pmatrix} \\ \iff & \frac{q_3 p_1}{q_3 p_2} = \frac{q_2 p_2}{q_2 p_3} = \frac{q_1 p_3}{q_1 p_0}, \quad \frac{q_3 p_1}{q_3 p_3} = \frac{q_2 p_2}{q_2 p_0} = \frac{q_1 p_3}{q_1 p_1}, \quad \frac{q_3 p_1}{q_3 p_0} = \frac{q_2 p_2}{q_2 p_1} = \frac{q_1 p_3}{q_1 p_2} \\ \iff & p_0 = p_1 = p_2 = p_3. \end{aligned}$$

Similarly, $p_0 = p_1 = p_2 = p_3$ is obtained for each of $q_1 = 0, q_2 = 0, q_3 = 0$.

Suppose two of q_0, q_1, q_2, q_3 are zero. If $q_0 = q_1 = 0$, we consider the rows' identity in the following S .

$$\begin{aligned} S &= \begin{pmatrix} 0 & 0 & q_3 p_1 / C_0 & q_2 p_2 / C_0 \\ 0 & 0 & q_3 p_2 / C_1 & q_2 p_3 / C_1 \\ 0 & 0 & q_3 p_3 / C_2 & q_2 p_0 / C_2 \\ 0 & 0 & q_3 p_0 / C_3 & q_2 p_1 / C_3 \end{pmatrix} \\ \iff & \frac{q_3 p_1}{q_3 p_2} = \frac{q_2 p_2}{q_2 p_3} \text{ and } \frac{q_3 p_1}{q_3 p_3} = \frac{q_2 p_2}{q_2 p_0} \text{ and } \frac{q_3 p_1}{q_3 p_0} = \frac{q_2 p_2}{q_2 p_1} \\ \iff & p_0 = p_1 = p_2 = p_3 \end{aligned}$$

Similarly, $p_0 = p_1 = p_2 = p_3$ is obtained for each of $q_1 = q_2 = 0, q_2 = q_3 = 0, q_3 = q_0 = 0$. For $q_0 = q_2 = 0$, we consider

$$S = \begin{pmatrix} 0 & q_3 p_1 / C_0 & 0 & q_1 p_3 / C_0 \\ 0 & q_3 p_2 / C_1 & 0 & q_1 p_0 / C_1 \\ 0 & q_3 p_3 / C_2 & 0 & q_1 p_1 / C_2 \\ 0 & q_3 p_0 / C_3 & 0 & q_1 p_2 / C_3 \end{pmatrix}.$$

The identity of the 0th row and the cyclically 0 or 2 left-shifted 2nd row, the identity of the 1th row and the cyclically 0 or 2 left-shifted 3rd row and the identity of the 0th row and the cyclically 0 or 2 left-shifted 1st row give the following constraints respectively.

$$\begin{aligned} & \left(\frac{q_3 p_1}{q_3 p_3} = \frac{q_1 p_3}{q_1 p_1} \text{ or } \frac{q_3 p_1}{q_1 p_1} = \frac{q_1 p_3}{q_3 p_3} \right) \text{ and } \left(\frac{q_3 p_2}{q_3 p_0} = \frac{q_1 p_0}{q_1 p_2} \text{ or } \frac{q_3 p_2}{q_1 p_2} = \frac{q_1 p_0}{q_3 p_0} \right) \text{ and} \\ & \left(\frac{q_3 p_1}{q_3 p_2} = \frac{q_1 p_3}{q_1 p_0} \text{ or } \frac{q_3 p_1}{q_1 p_0} = \frac{q_1 p_3}{q_3 p_2} \right) \\ & \iff (p_1 = p_3 \text{ or } q_1 = q_3) \text{ and } (p_0 = p_2 \text{ or } q_1 = q_3) \\ & \quad \text{and } (p_1/p_2 = p_3/p_0 \text{ or } q_3 p_1 / q_1 p_0 = q_1 p_3 / q_3 p_2) \\ & \iff (p_1 = p_3 \text{ and } p_0 = p_2) \text{ or } (q_1 = q_3 \text{ and } P_2). \end{aligned}$$

Similarly, $q_1 = q_3 = 0 \iff (p_1 = p_3 \text{ and } p_0 = p_2) \text{ or } (q_0 = q_2 \text{ and } P_2)$.

Suppose three of the q_0, q_1, q_2, q_3 are zero.

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Under $g(Y) = i$ cyclically shifting i steps left every i -th row, the three rows in R become identical.

The sufficiency of the conditions for all cases is easily confirmed by substituting the conditions into R . ■

Appendix D. Proof of Theorem 1

(1) When $q_0, \dots, q_{m-1} > 0$.

Let $R = (r_{k,i})$ be a $m \times m$ matrix such that $r_{k,i} = \frac{p_i q_{k-i}}{C_k}$ where $C_k = \sum_{i=0}^{m-1} p_i q_{k-i} \neq 0$ because $p_0, \dots, p_{m-1} > 0$ and $\sum_{j=0}^{m-1} q_j = 1$. We assume

that for the reversibility there exist $g(k)$ ($k = 0, \dots, m-1$) so that a shift of every row k to the left by $g(k)$ respectively in R derives a matrix T where all the rows are identical.

If T has two rows such that

$$(p_i q_j / C_{i+j}, p_{i+1} q_{j-1} / C_{i+j}, \dots, p_{i-1} q_{j+1} / C_{i+j})$$

$$(p_i q_k / C_{i+k}, p_{i+1} q_{k-1} / C_{i+k}, \dots, p_{i-1} q_{k+1} / C_{i+k})$$

for some indeces i, j, k , then $q_{j+l} / C_{i+j} = q_{k+l} / C_{i+k}$ for $l = 0, 1, \dots, m-1$. This implies $\sum_{l=0}^{m-1} q_{j+l} / C_{i+j} = \sum_{l=0}^{m-1} q_{k+l} / C_{i+k}$. Thus, $C_{i+j} = C_{i+k}$ holds because $\sum_{l=0}^{m-1} q_{j+l} = \sum_{l=0}^{m-1} q_{k+l} = 1$. Accordingly, $q_{j+l} = q_{k+l}$ holds for $l = 0, 1, \dots, m-1$, which means $q_{k+a} = q_k$ for all $k = 0, \dots, m-1$ and some a dividing m . On the other hand, if there exist a dividing m such as $q_{k+a} = q_k$ for all $k = 0, \dots, m-1$, then there exist $g(k)$ ($k = 0, \dots, m-1$) making T have two rows mentioned above (if T does not have such two rows, $q_{k+a} = q_k$ for all $k = 0, \dots, m-1$ hold only for $a := m$).

Similarly, if T has two rows such that

$$(q_j p_i / C_{j+i}, q_{j-1} p_{i+1} / C_{j+i}, \dots, q_{j+1} p_{i-1} / C_{j+i})$$

$$(q_j p_k / C_{j+k}, q_{j-1} p_{k+1} / C_{j+k}, \dots, q_{j+1} p_{k-1} / C_{j+k})$$

for some indeces i, j, k , then $p_{i+l} = p_{k+l}$ for $l = 0, 1, \dots, m-1$, which means $p_{k+b} = p_k$ for all $k = 0, \dots, m-1$ and some b dividing m (if T does not have such two rows, $p_{k+b} = p_k$ for all $k = 0, \dots, m-1$ hold only for $b := m$).

We notice that $\min\{a, b\}$ divides $\max\{a, b\}$ since m is a power of some prime number, and that $\max\{a, b\}$ divides m by the definitions. Assume the chosen a, b are the smallest satisfying the above properties. Because the values of $\{p_i\}$ and $\{q_j\}$ have cycles of a and b , respectively, R consists of identical $a \times b$ submatrices. Accordingly, we focus on one of the submatrices which is sufficient for our proof.

Let $R = (r_{k,i})$ be such that $r_{k,i} = \frac{p_i q_{k-i}}{C_k}$ and $C_k = \sum_{i=0}^{m-1} p_i q_{k-i}$, and we assume that T has been obtained by shifting row k left by $g(k)$ columns in R so that all the rows are identical in T .

If two rows in T are

$$(p_i q_j / C_{i+j}, p_{i+1} q_{j-1} / C_{i+j}, \dots, p_{i-1} q_{j+1} / C_{i+j})$$

$$(p_i q_k / C_{i+k}, p_{i+1} q_{k-1} / C_{i+k}, \dots, p_{i-1} q_{k+1} / C_{i+k})$$

for some indeces i, j, k , then $q_{j+l} = q_{k+l}$ for $l = 0, 1, \dots, m-1$, which means $q_{k+a} = q_k$ for some a dividing m , else $a := m$. On the other hand, if two rows in T are

$$(q_i p_j / C_{i+j}, q_{i-1} p_{j+1} / C_{i+j}, \dots, q_{i+1} p_{j-1} / C_{i+j})$$

$$(q_i p_k / C_{i+k}, q_{i-1} p_{k+1} / C_{i+k}, \dots, q_{i+1} p_{k-1} / C_{i+k})$$

for some indeces i, j, k , then $p_{j+l} = p_{k+l}$ for $l = 0, 1, \dots, m-1$, which means $p_{k+b} = p_k$ for some b dividing m , else $b := m$.

We notice that $\min\{a, b\}$ divides $\max\{a, b\}$, and $\max\{a, b\}$ divide m , and assume the chosen a, b are the smallest satisfying the above properties.

Suppose $a \leq b$. In matrix

$$R = \begin{pmatrix} p_0 q_0 / C_0 & p_1 q_{a-1} / C_0 & \cdots & p_{b-1} q_1 / C_0 \\ p_0 q_1 / C_1 & p_1 q_0 / C_1 & \cdots & p_{b-1} q_2 / C_1 \\ \cdots & \cdots & \cdots & \cdots \\ p_0 q_{a-1} / C_{a-1} & p_1 q_{a-2} / C_{a-1} & \cdots & p_{b-1} q_0 / C_{a-1} \end{pmatrix},$$

if we do not shift row 1 to compare with row 0 in R , we obtain $q_0 = \dots = q_{a-1}$; and if we shift row 1 right by $j \neq 0$ columns to compare with row 0, we obtain for $u = 0, \dots, a-1$

$$\frac{p_{j+u} q_{a-j-u}}{p_u q_{1-u}} = \frac{p_{j+u+a} q_{-j-u}}{p_{u+a} q_{1-u-a}}.$$

which means for $u = 0, 1, \dots, b-1$,

$$\frac{p_{u+a}}{p_u} = \frac{p_{j+u+a}}{p_{j+u}} = \dots = \frac{p_{u-j+a}}{p_{u-j}} = \dots.$$

By multiplying all the terms, we find that $\frac{p_{u+a}}{p_u} = 1$ for $u = 0, 1, \dots, b-1$.

If $b \leq a$, we similarly find that $\frac{q_{u+b}}{q_u} = 1$ for $u = 0, 1, \dots, a-1$. So, we only need to consider R of size $d \times d$ with $d := \{a, b\}$, and may assume that there will be no nontrivial relation among $\{p_i\}, \{q_j\}$, which means that there will be no conflict among indeces.

We complete this proof if we show either $p_0 = \dots = p_{d-1}$ or $q_0 = \dots = q_{d-1}$, which means $p_0 = \dots = p_{m-1}, q_0 = \dots = q_{m-1}$. However, we see that $\prod_{j=0}^{d-1} t_{i,j} = \frac{1}{C_{i+j}^d} \prod_{u=0}^{d-1} p_u \prod_{v=0}^{d-1} q_v$, for $T = (t_{i,j})$. Since $\frac{t_{0,j}}{t_{0,k}} = \frac{t_{1,j}}{t_{1,k}} = \dots = \frac{t_{d-1,j}}{t_{d-1,k}} =$

C and $1 = \prod_{i=0}^{d-1} \frac{t_{i,j}}{t_{i,k}} = C^d$, we have $\frac{t_{i,j}}{t_{i,k}} = C = 1$ for $k = 0, \dots, d-1$. On the other hand, since $\prod_{k=0}^{d-1} \frac{t_{i,j}}{t_{i,k}} = t_{i,j}^d / \{ \frac{1}{C_{i+j}^d} \prod_{u=0}^{d-1} p_u \prod_{v=0}^{d-1} q_v = 1 \}$, we have $t_{i,j} = \frac{1}{C_{i+j}} [\prod_{u=0}^{d-1} p_u \prod_{v=0}^{d-1} q_v]^{1/d}$ for all $i, j = 0, \dots, d-1$. Thus, $p_i q_j = [\prod_{u=0}^{d-1} p_u \prod_{v=0}^{d-1} q_v]^{1/d}$ for all $i, j = 0, \dots, d-1$, which means $p_i = q_j = d[\prod_{u=0}^{d-1} p_u \prod_{v=0}^{d-1} q_v]^{1/d}$ for all $i, j = 0, \dots, d-1$.

In any case, $p_0 = \dots = p_{m-1}$ or $q_0 = \dots = q_{m-1}$ if $q_0, \dots, q_{m-1} > 0$.

(2) When $q_j = 0$ for some j . For each k such that $q_k > 0$, we select columns $k, k+c, \dots, k+m-c$ in S to obtain the matrix of size $m \times \frac{m}{c}$

$$S_k := \begin{pmatrix} \frac{q_k p_{-k}}{C_0} & \frac{q_{k-c} p_{-k+c}}{C_0} & \dots & \frac{q_{k+c} p_{-k-c}}{C_0} \\ \frac{q_k p_{-k+1}}{C_1} & \frac{q_{k-c} p_{-k+1+c}}{C_1} & \dots & \frac{q_{k+c} p_{-k+1-c}}{C_1} \\ \dots & \dots & \dots & \dots \\ \frac{q_k p_{-k+m-1}}{C_{m-1}} & \frac{q_{k-c} p_{-k+m-1+c}}{C_{m-1}} & \dots & \frac{q_{k+c} p_{-k+m-1-c}}{C_{m-1}} \end{pmatrix}.$$

Furthermore, for each $j = 0, 1, \dots, c-1$, we select rows $j, j+c, \dots, j+m-c$ in S_k to obtain the matrix of size $\frac{m}{c} \times \frac{m}{c}$

$$S_{jk} := \begin{pmatrix} \frac{q_k p_{j-k}}{C_0} & \frac{q_{k-c} p_{j-k+c}}{C_0} & \dots & \frac{q_{k+c} p_{j-k-c}}{C_0} \\ \frac{q_k p_{j-k+c}}{C_1} & \frac{q_{k-c} p_{j-k+2c}}{C_1} & \dots & \frac{q_{k+c} p_{j-k}}{C_1} \\ \dots & \dots & \dots & \dots \\ \frac{q_k p_{j+m-k-c}}{C_{m-1}} & \frac{q_{k-c} p_{j+m-k}}{C_{m-1}} & \dots & \frac{q_{k+c} p_{j+m-k-2c}}{C_{m-1}} \end{pmatrix}.$$

Since S_{jk} is a square matrix and all the elements are positive, for reversibility, the condition

$$p_j = p_{j+c} = \dots = p_{j+m-c} \text{ or } q_k = q_{k+c} = \dots = q_{k+m-c}$$

for all $j = 0, 1, \dots, c-1$ and $k = 0, 1, \dots, c-1$ (for k such that $q_k = 0$, the condition is trivially true) is required, i.e., either

1. $p_j = p_{j+c} = \dots = p_{j+m-c}$ for $j = 0, 1, \dots, c-1$, or
2. $q_k = q_{k+c} = \dots = q_{k+m-c}$ for $k = 0, 1, \dots, c-1$

is necessary. It remains to prove that if either of the two condition is satisfied, reversibility holds. Under the first condition, S_k is a uniform matrix, and expresses reversibility. Under the second condition, in S_k consisting of $\{p_l\}$, the i th and j th rows coincide each other by shifting if $|i - j|$ is divided by c . Hence, the condition that S_k expresses reversibility is equivalent to P_c under the second condition. ■

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